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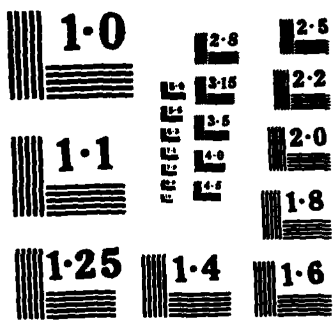

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FINAL SUMMARY REPORT, 1975 - 1985

High Temperature Gas Energy Transfer

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OFFICE OF NAVAL RESEARCH

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Work under this contract is summarized.

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I. SUMMARY OF WORK ACCOMPLISHED

A. THEORY AND METHODS

1. Development of a new method called the Diffusion Cloud Method for the study of intermolecular vibrational energy transfer in reacting unimolecular systems. The method is an extension, both of theory and experimental technique, of the Polanyi Diffusion Flame Method for the study of fast bimolecular reactions. Thermal systems may be studied both in the transient and in the steady state regimes.

2. Development of the theory and method of a new technique called the Variable Encounter Method for the study of sequential vibrational energy transfer between gas molecules and hot surfaces, at the level of energy corresponding to the region above the critical threshold for reaction E_0. Application has been made to many molecules.

3. A critique of the exact vibrational state computational algorithm of Beyer-Swinehart-Stein-Rabinovitch was given.

4. A theoretical illustration of a model for V-T,R vibrational energy transfer restricted by angular momentum conservation was given.

5. Theoretical treatment of a Boltzmann strong collision model has led to generalizations on energy transfer efficiency as a function of both molecule size, ambient temperature and hot molecule energy level. Correlation has been made between various average energy transfer quantities ($\langle \Delta E \rangle_{all}$ and $\langle \Delta E \rangle_{down}$) for step-ladder and exponential forms of the collisional transition probability matrix, P.

B. EXPERIMENTAL FINDINGS

1. The collisional efficiency of fused silica and pyrex surface for energy transfer has been studied over a wide range of temperatures for a variety of molecules and found to decrease with rise of temperature. Efficiency approaches strong collider behavior at lower temperatures. The importance of the attractive potential interaction is emphasized.

2. Homogeneous studies on energy transfer between a polyatomic molecule and various bath gases at high temperatures also corroborate a decrease in efficiency with rise of temperature. The decline in efficiency itself decreases at very high temperatures suggesting a possible switch to a dominant Landau-Teller repulsive form at still higher temperatures.

3. Correlations have been found between collision transfer efficiency and molecular structure parameters. In general, efficiency declines with molecule heat bath size (eigenstate density) and increases with polarity of the molecule . Apart from a propensity for more complex reaction mechanisms and catalytic behavior, the energy transfer properties of energetic materials at a surface seem to follow just the behavior expected form the intermolecular potential and not that of the intramolecular or reaction potential. More stable molecules can thus suffice to delineate the energy transfer properties expected for energetic materials.

4. The transient region of energy accommodation in thermal systems have been studied for the first time for polyatomic molecules; mean first passage times have been measured.

5. The form of the collisional transition probability matrix has been investigated; favored analytic functional forms have been found and others excluded.

6. The study of gas/surface energy transfer has been extended to metals. Gold surfaces are stronger energy transfer media than fused silica. they behave as ideal strong collision agents at lower temperatures.

7. Liquid metal surfaces (tin and gallium) also display high efficiency for vibrational energy transfer. No discontinuity in efficiency appears at the melting point of tin.

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